Russian Journal of Organic Chemistry 2014 vol.50 N4, pages 459-463

Structure-reactivity relationships in terms of the condensed graphs of reactions

Madzhidov T., Polishchuk P., Nugmanov R., Bodrov A., Lin A., Baskin I., Varnek A., Antipin I.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

An approach for the prediction of rate constants of chemical reactions, based on the representation of a chemical reaction as a condensed graph, has been tested on more than 1000 bimolecular nucleophilic substitution reactions with neutral nucleophiles in 38 solvents. Molecular fragment descriptors, temperature, and solvent parameters characterizing solvation power have been used in the reaction modeling. The obtained models ensure a good correlation between the predicted and experimental values; the corresponding deviations are comparable with interlaboratory measurement errors. © 2014 Pleiades Publishing, Ltd.

http://dx.doi.org/10.1134/S1070428014040010